

# Modeling Solute Transport in Streams with Pools and Riffles: Storage-Sorption Model

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## 1. RESEARCH BACKGROUND AND OBJECTIVES

Flow and mixing characteristics in real streams are substantially different from those observed in uniform channels. Boundary geometry of natural streams is not smooth and regular. Every irregularity contributes to mixing of pollutants. Characteristics of low flows in natural streams are substantially different from those observed at bank-full or flood stages. Under low flow conditions, pollution problems are most acute. The water quality of streams receiving municipal, industrial, and agricultural return flow is further degraded when natural streamflow is low. Dilution of contaminants decreases as streamflow decreases; thus the hazard associated with an accidental spill may be much greater at low flow than at a higher flow. Variations in bed geometry such as pool and riffle structure, dominant channel features during low flow (Leopold et al., 1964), play their strongest role in affecting mixing characteristics of polluted releases in the channel. Under low flow conditions, irregularities and unevenness along the streams caused by pools and riffles, which are dominant channel features at low flow, can create storage zones which have significant storage effects.

During prolonged periods of low flow, slow water movement at pool and the absence of sediment transport enhance sorption onto the relatively immobile bed sediment to become a major control on solute transport. Therefore, in natural channels under low flow conditions during which pollutants have repeated opportunity for contact with relatively immobile bed materials and which irregularities and unevenness caused by pools and riffles create storage zones which have significant storage effects, pollutant transport is determined by the interaction of physical and chemical processes. In natural streams, among the physical processes, mass storage and exchange mechanisms are important along with mean flow advection and shear flow dispersion, among the chemical processes, sorption and desorption mechanisms are mostly important

The one-dimensional (1-D) Fickian-type dispersion equation derived by Taylor (1954) has been widely used to give a reasonable estimate of the rate of longitudinal dispersion in uniform channels. Although analytical solutions of the 1-D Fickian dispersion equation with given initial and boundary conditions are easy to obtain, the use of the 1-D dispersion equation has several limitations. An immediate limitation is that the Fickian dispersion model cannot be applied until after the initial period, i.e., the model should be limited to locations far downstream from the source at which the balance between advection and diffusion assumed by Taylor is reached (Fischer et al., 1979). Fischer (Fischer et al., 1979) reasoned that during the early period of the transport process, the advective transport due to the velocity distribution is dominant. During this so-called "initial period" advection and diffusion are by no means in balance, and Taylor's analysis does not apply. He also reasoned that because of the dominant effect of the velocity distribution during the initial period, the longitudinal distribution of the cross-sectionally averaged concentration is highly skewed, with a steep gradient in the downstream direction and a long tail in the upstream direction. The skewness increases during the initial period of transport, reaches a maximum, and then begins to decrease as the concentration distribution tends toward symmetry at asymptotically large times. The longitudinal variance of the concentration distribution increases non-linearly with time during

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the initial period, and during the later or so-called "Fickian (Taylor) period," the variance increases linearly for steady, uniform flow.

However, literature describing field studies (Godfrey and Frederick, 1970; and Avanzino et al., 1984) shows that concentration distribution data collected in natural streams show non-linear behavior of the variance for times beyond the initial period. Furthermore, most experimental studies in natural streams have produced concentration-time curves significantly more skewed than the concentration distribution predicted by the solution of the 1-D dispersion equation. These show that water and dye are retained in the regions having storage effects along the channel bed and banks and then released slowly after the main cloud has passed. Several investigators have suggested that a complete analysis must include the effect of channel storage zones (Hays et al., 1966; Bencala, 1983; Jackman et al., 1984). They demonstrated that their models incorporating the storage effect along the channel bed and banks, the so-called "dead zone models," can describe the dispersion process in natural channels better than the 1-D dispersion model. In more recent years, Seo (1990) and Seo and Maxwell (1992) have conducted important research on the transport and mixing characteristics for pollutants discharged into natural streams with pools and riffles. They showed that in natural channels under low flow conditions, the effect of storage induced by the pool-riffle sequences should be considered adequately in the modeling of transport and mixing of conservative solutes.

The objective of the present study was to develop a mathematical model to predict adequately complex mixing characteristics of sorptive pollutants in natural streams under low flow conditions. Sorption of pollutants onto the bed sediment as well as mass storage and exchange in the storage zones were incorporated into the one-dimensional mass balance equations to make model equations as coupled quasi-two-dimensional transport equations. Dispersion data from stream experiments were used to test and verify the proposed mathematical model. The predicted concentration-time curves were compared to the measured stream data.

## **2. MODEL DEVELOPMENT**

### **2.1 Conceptual Model**

In this model a typical cross section is considered to consist of two distinct zones, a flow zone and a storage zone. In the flow zone, the dominant mass transport mechanisms are longitudinal advection and dispersion. The storage zones are considered as regions having vortex or recirculating flow and having mass interchange with the main flow across the interface between the flow and the storage zones. The storage zones serve to retain part of the solute as the main cloud passes, and the solute is then slowly released back into the flow zone. Among several conceptually different physical models of the transient storage of mass in the storage zone (Jackman et al. 1984), the exchange model assumes a different uniform concentration in each zone. Mass transfer at the interface between the zones is considered to be proportional to the difference in the average concentrations.

Several models were developed to describe sorption and desorption mechanisms (Kim et al., 1990). Sorption accounts for binding of the dissolved pollutant molecules or ions onto the bed sediment of the stream bed whereas desorption accounts for the release of solute back to the water column of the stream. Among those models, Michaelis-Menten isotherm, Freundlich isotherm, and linear isotherm were tested in the preliminary investigation of sorption models in this study. Michaelis-Menten isotherm, in which maximum uptake rate and half-saturation constants are used as parameters, gives the most stable results with widely varying dissolved concentration among others. Freundlich isotherm which assumes that sorption rate is proportional to  $(1-N)$  power of dissolved concentration is better suited in describing sorption for narrow concentration range. Linear isotherm which has the simplest form is easy to estimate sorption parameters. In the Storage-Sorption Model developed in this study, sorption and desorption mechanisms have been considered using linear isotherm, which is the first-order mass transfer model. This model relates the rate of change of concentration of the

sorbing element on the sediment to the difference between the concentration of that element and its potential equilibrium concentration in the stream. In this submodel, distribution coefficient  $k_d$ , which means partitioning of the contaminant between the liquid and solid phases at equilibrium, is assumed to be constant (Bencala et al., 1983). In general, the sediment particles on which sorption of toxic components occurs may be either organic or inorganic, i.e. suspended and bed sediment and biota or benthos. However, in this study emphasis is on the sorption mechanisms of toxic heavy metals onto inorganic bed sediment.

## 2.2 Mathematical Model

The equations describing the Storage-Sorption Model are derived using conservation of mass. The mass balance equation in the flow zone for steady flow is

$$A_f \frac{\partial C}{\partial t} = -U_f A_f \frac{\partial C}{\partial x} + \frac{\partial}{\partial x} \left( A_f K \frac{\partial C}{\partial x} \right) - Pk(C - S) + A_f k_d \rho_f \lambda_f \left( \frac{1}{k_d} C_B - C \right) \quad (1)$$

in which  $A_f$  = cross-sectional area of the flow zone;  $C$  = the concentration of mass in the flow zone;  $U_f$  = flow zone velocity;  $K$  = dispersion coefficient;  $P$  = wetted contact length between the flow zone and the storage zone in the transverse or vertical direction;  $k$  = mass exchange coefficient;  $S$  = the concentration of mass in the storage zone;  $k_d$  = distribution coefficient;  $\rho_f$  = accessible sediment density in the flow zone which is the mass of the sediment on the streambed in effective contact with a given volume of water in the stream;  $\lambda_f$  = first-order rate coefficient for sorption/desorption in the flow zone;  $C_B$  = sorbate concentration on the flow zone streambed sediment;  $t$  = time; and  $x$  = distance. A mass balance equation describing concentration of sorbed pollutants on the flow zone streambed sediment is

$$\frac{\partial C_B}{\partial t} = -\lambda_f (C_B - k_d C). \quad (2)$$

A mass balance equation describing concentration dissolved solutes in the storage zone is

$$A_s \frac{\partial S}{\partial t} = Pk(C - S) + A_s k_d \rho_s \lambda_s \left( \frac{1}{k_d} S_B - S \right) \quad (3)$$

in which  $A_s$  = cross-sectional area of the storage zone perpendicular to the general flow direction;  $\rho_s$  = accessible sediment density in the storage zone;  $\lambda_s$  = first-order rate coefficient for sorption/desorption in the storage zone; and  $S_B$  = sorbate concentration of the sediment associated with the storage zone. A mass balance equation describing concentration of sorbed pollutants on the storage zone sediment is

$$\frac{\partial S_B}{\partial t} = -\lambda_s (S_B - k_d S). \quad (4)$$

If the pollutants is released with constant concentration for a limited period, the initial conditions for the Dirichlet-type are

$$C(0, x) = 0, \quad x > 0 \quad (5a)$$

$$C(t, 0) = C_0, \quad 0 < t \leq \tau \quad (5b)$$

$$C(t, 0) = 0, \quad t > \tau \quad (5c)$$

in which  $C_0$  = initial concentration injected;  $\tau$  = period of injection. The Dirichlet-type boundary conditions for an infinite domain are

$$C(t, \pm\infty) = 0. \quad (6)$$

If the pollutant is initially released into only the flow zone so that there is no concentration in the storage zone, the initial condition of Dirichlet-type for the storage zone is

$$S(0, x) = 0 \quad (7)$$

and the boundary conditions for the infinite domain are

$$S(t, \pm\infty) = 0. \quad (8)$$

The initial and boundary conditions for the sorbate on the sediment associated with both the flow and storage zones are obtained under the assumption that the pollutant is initially released into only the water column of the flow zone so that there is no concentration in the sorbate on the sediment associated with both the flow and storage zones. For the sorbate on the sediment of the flow zone, this assumption results

$$C_B(0, x) = 0 \quad (9a)$$

$$C_B(t, \pm\infty) = 0. \quad (9b)$$

For the sorbate on the sediment of the storage zone, this assumption results

$$S_B(0, x) = 0 \quad (10a)$$

$$S_B(t, \pm\infty) = 0. \quad (10b)$$

## 2.3 Numerical Modeling

An analytical solution of the given sets of governing equations (Eqs. 1-4) corresponding to the initial and boundary conditions (Eqs. 5-10) was not available because of the non-uniform parameters and the existence of the mass exchange term and sorption term in the equation. Therefore, numerical techniques were applied to solve the given sets of governing equations. Furthermore, given sets of the working equations consist of four equations describing coupled solute transport in the flow zone, sorption onto the flow zone streambed sediment, solute transport and sorption in the storage zone, and sorption onto the storage zone sediment. The equations describing mass balance of the solute in two zones are interrelated by mass exchange term modeling the storage processes. The equations describing mass balance of the sorbate on the sediment in each zone are coupled directly to the equations describing mass balance of the solute in each zone. In this study, combined procedure of the analytical solution of one of the sorbate equations and iteration method for solution of remaining three equations was used to solve complex sets of coupled working equations. Detailed procedure is as follows: First, Eq. 4 was solved analytically to get a explicit solution of  $S_B$  in which solute concentration in the storage zone,  $S$  is numerically integrated using simple trapezoidal rule. The solution of  $S_B$  was inserted in Eq. 3 to reduce one unknown dependent variable. Second, guessed value of  $C$  was

used in solving Eqs. 2 -3 numerically to obtain  $C_B$  and  $S$ . Then, Eq. 1 could be solved to obtain  $C$  with the known values of  $C_B$  and  $S$ . This process was iterated until the differences between computed and guessed concentrations of  $C$  are within the specified tolerance.

For the second stage of solution procedure, among the various types of numerical schemes tested by Seo (1990), the finite difference method (FDM) developed by Stone and Brian (1963) was selected to solve the remaining three equations. This method, based on the Crank-Nicholson implicit approach, was considered to have no stability limitations as in the cases of other implicit schemes. The truncation error involved in this scheme was considered to be  $O(\Delta t^2 + \Delta x^2)$ , as in other Crank-Nicholson implicit approaches with the central difference approximation for space discretization, which is a higher-order than that of a fully implicit approach,  $O(\Delta t + \Delta x^2)$ .  $\Delta t$  is the time increment and  $\Delta x$  is the distance step. The time derivative  $\partial C/\partial t$  of the flow zone equation was represented by the spread form backward time difference approximation. The advective term was discretized by using the Crank-Nicholson approach, in which  $\partial C/\partial x$  was centrally differenced. The dispersive term was also discretized by using the Crank-Nicholson type implicit method. Substituting each term into Eq. 1, and expanding the resulting equation for all the nodal points along the  $x$  axis, a set of simultaneous linear algebraic equations, of which the coefficient matrix is tridiagonal, can be obtained. The resulting system of algebraic equations was solved by using the Thomas algorithm, a variation of Gaussian elimination. The storage zone equation and sorbate equation were also discretized by using the FDM developed by Stone and Brian similar to the flow zone equation.

### 3. MODEL APPLICATIONS

#### 3.1 Stream Data

The Storage-Sorption Model developed in this study was tested by using field data measured by Avanzino et al. (1984). Avanzino et al. described the dispersion study of conservative and nonconservative tracers in a small stream, Uvas Creek in California, U.S.A. As shown in Fig. 1, the channel is highly irregular. It is composed of alternating pools and riffles and pool frequency ranges mostly 6 to 7 channel widths which falls into the range of that of the natural pool-riffle sequences studied by other investigators (Leopold et al., 1964). The experiment was conducted in late summer during a period of low flow ( $Q = 0.0125 \text{ m}^3/\text{s}$ ). The strontium tracer, as a sorptive pollutant, was injected at a constant rate for three hours and reached a maximum concentration of 1.73 mg/l a short distance below the injection point. Background concentration was measured to be 0.13 mg/l. In addition to the intense monitoring of in-stream concentration of strontium, some of sorbed strontium concentrations on bed sediments was measured.

#### 3.2 Simulation Results

Laboratory experiment and field observation in pool-and-riffle streams (Bencala, et al., 1983; Seo, 1990) show that the parameters most likely to vary spatially are storage zone submodel parameters and sorption submodel parameters as well as flow depth and velocity. These values could be considerably different in pool versus riffle sections. In the numerical model, the simplified geometric and hydraulic characteristics of the pool-riffle sequences were used. The simplified pool-riffle sequences was determined based on the geomorphologic theory proposed by Leopold et al. (1964) and verified by many researchers in natural streams. Schematic diagram of the simplified pool-riffle sequences is depicted in Fig. 2.

The nonuniform hydraulic parameters, such as the flow depth and the storage zone area ratio, were considered to have single constant values at the pool and riffle, and then to vary linearly through the transition between the pool and the riffle. The mass exchange coefficient and accessible mass density were also considered to follow the above assumption, but the dispersion coefficient, sorption rate coefficient, and distribution coefficient were assumed to be

constant through the whole reach of pool-riffle sequences. The model parameters used for simulation are presented in Table 1. All the sorption parameters except accessible mass density were selected from independently-decided values by measurements (Bencala et al., 1983). The other model parameters were estimated by empirical relationships proposed by several researchers including Bencala (1983) and Seo (1990).

TABLE 1.-Summary of the Model Parameters Used in the Simulation

	$A_s/A$ (m)	Depth (m <sup>2</sup> /s)	K	k (m/s)	$k_d$ (ml/g)	$\rho_f$ (g/m <sup>3</sup> )	$\rho_s$ (g/m <sup>3</sup> )	$\lambda_f$ (1/s)	$\lambda_s$ (1/s)
Pool	0.49	0.30		$1.2 \cdot 10^{-4}$		$0.14 \cdot 10^5$	$0.14 \cdot 10^5$		
Riffle	0.35	0.05		$0.2 \cdot 10^{-4}$		$0.14 \cdot 10^4$	$0.14 \cdot 10^4$		
Avg.	0.43	0.20	0.21	$0.86 \cdot 10^{-4}$	70.0	$0.09 \cdot 10^5$	$0.09 \cdot 10^5$	$0.3 \cdot 10^{-4}$	$0.48 \cdot 10^{-3}$

Comparisons of the concentration-time curves of the model simulations with those obtained in the stream experiments are depicted in Fig. 3. In general, in overall shape, the concentration-time curves given by the storage zone model excellently fit the measured concentration-time curves, whereas those predicted by conventional 1-D dispersion model usually fail to fit. The tails of the concentration-time curves by the storage zone model are quite close to those of the measured concentration-time curves. The peak concentrations predicted by the Storage-Sorption Model are quite close to the experimental data. The model also predicts the elapsed times to peak concentration very accurately. In Fig. 3, concentrations are also compared for simulations with parameters of pool-and-riffle streams and parameters of uniform channels in which average value of the parameters of the pool-and-riffle sequences are used. In overall shape and peak concentration, simulations with parameters of pool-and-riffle streams better fit the measured data than simulations with parameters of uniform channels. The result demonstrates the differences between transport in pool-and-riffle streams versus transport in more uniform channels.

In addition to comparisons of dissolved solute concentration, concentrations of sorbate on the sediment are also compared for simulations with parameters of pool-and-riffle streams and parameters of uniform channels in which average value of the parameters of the pool-and-riffle sequences are used. These comparisons are depicted in Fig. 4. Both simulation results show that there is a moderate agreements with measured sorbate data of sediment of two different sizes in time to peak and in the persistence of the tails. Simulations with parameters of pool-and-riffle streams show the better fit to the measured data.

#### 4. CONCLUSIONS

The comparison between measured and predicted concentration curves by the Storage-Sorption Model shows that there is a good level of agreement in the general shape, peak concentration and time to peak. The proposed model shows improved behavior in predicting natural mixing processes in natural channels with pools and riffles.

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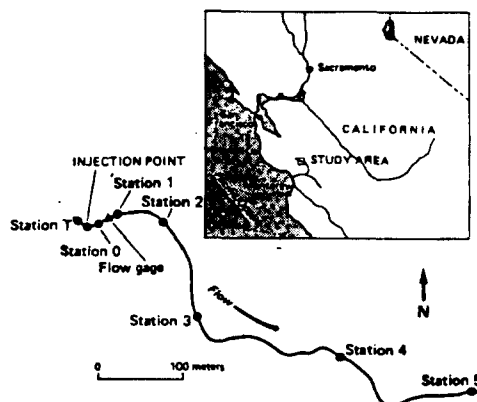


Fig. 1 Experimental Reach of Uvas Creek, Santa Clara County, California (after Avanzino et al., 1984)

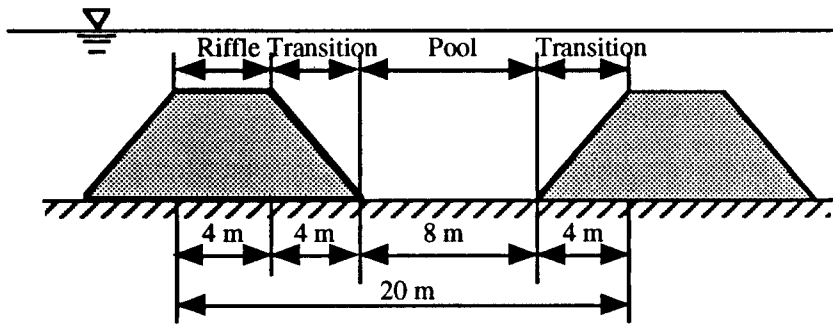


Fig. 2 Schematic Diagram of the Simplified Pool-Riffle Sequences

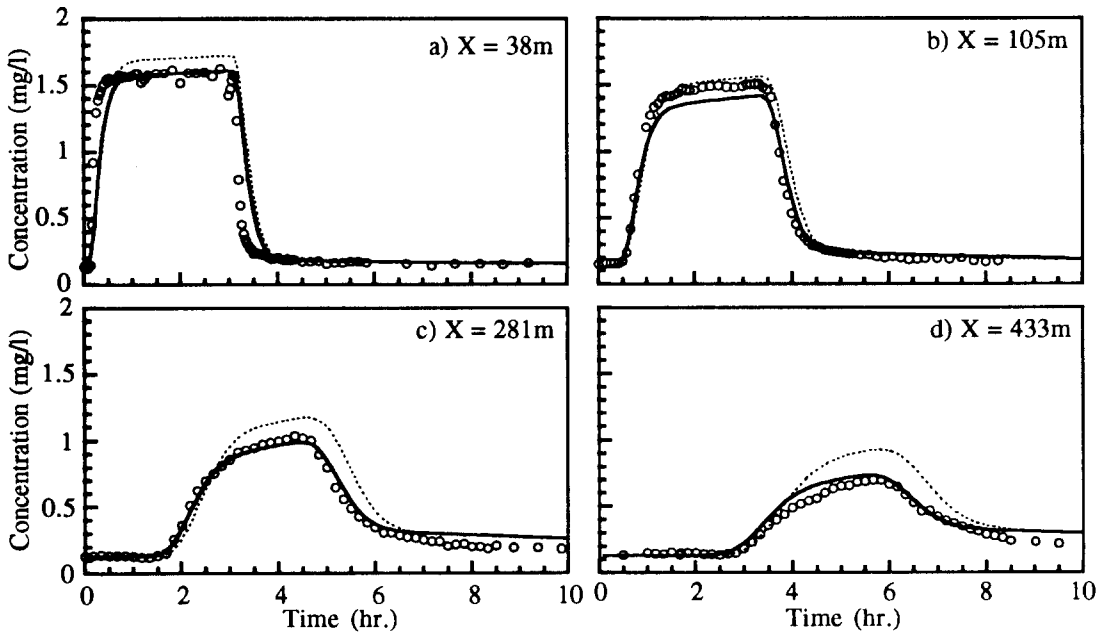


Fig. 3 Concentration Distribution of Observed Dispersion Data and Distributions Fitted by Storage-Sorption Model;  $\circ$  Observed Data; — Storage-Sorption Model with Parameters of Pool-Riffle Sequences; - - - - - Storage-Sorption Model with Parameters of Uniform Channels

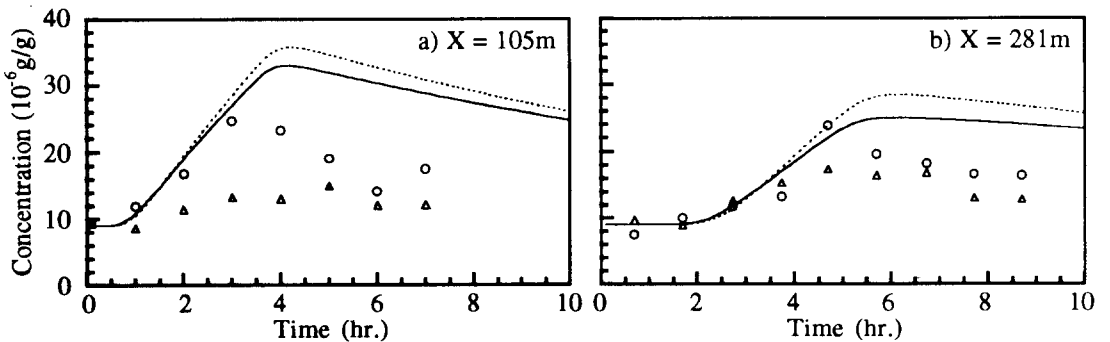


Fig. 4 Sorbate Concentration Distribution of Observed Data and Distributions Fitted by Storage-Sorption Model;  $\circ$  Observed Data (sediment size: 0.18~0.25mm);  $\triangle$  Observed Data (sediment size: 3.4~4.0mm); — Storage-Sorption Model with Parameters of Pool-Riffle Sequences; - - - - - Storage-Sorption Model with Parameters of Uniform Channels